

Abstract

The present invention concerns methods and systems for predicting the biological function(s) of proteins. The invention is based on the development of functional site descriptors for discrete protein biological functions. Functional site descriptors are geometric representations of protein functional sites in three-dimensional space, and can also include additional parameters, for example, conformational information. Following their development, one or more functional site descriptors (for one or more different biological functions) are used to probe protein structures to determine if such structures contain the functional sites described by the corresponding functional site descriptors. If so, the protein(s) containing the functional site(s) are predicted to have the corresponding biological function(s). In preferred embodiments, a library of functional site descriptors is used to probe inexact protein structures derived by computational methods from amino acid sequence information to predict the biological function(s) of such sequences and of the gene(s) encoding the same.